

Particle and Energy Transport in quantum disordered and quasi-periodic chains connected to mesoscopic Fermi reservoirs

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We study a model of nonequilibrium quantum transport of particles and energy in a many-body system connected to mesoscopic Fermi reservoirs (the so-called meso-reservoirs). We discuss the conservation laws of particles and energy within our setup as well as the transport properties of quasi-periodic and disordered chains.

§1. Introduction

Understanding the macroscopic transport from a microscopic point of view is a central topic of statistical physics. Especially, the development of nanoscale devices reveals unconventional transport. Thus, the study of transport in mesoscopic systems has significant value both in fundamental theory and for applications in future technologies. Since mesoscopic systems are strongly coupled with the environment, their understanding in nonequilibrium regimes requires knowledge of the global features of the total system including the environment (reservoirs). Recently, we proposed a model that comprises mesoscopic reservoirs with a finite number of degrees of freedom¹⁾ (the so-called meso-reservoirs), and study the transport properties of periodic chains. In particular, the parameter dependence of the transport properties as well as the Onsager reciprocity relation were studied.

In this paper, we study periodic chains in more detail, as well as quasi-periodic and disordered chains. We will also discuss the conservation law of energy and particles within our setup.

§2. Model

A key idea of our model is to enforce the finite reservoirs to equilibrium (or almost equilibrium) state using the Lindblad dissipator.^{2),3)} In particular, if the term in the Liouvillean evolution containing the Lindblad dissipator is small, we can interpret that the ‘traced-out-infinite-reservoirs’ (*super-reservoirs*) force our finite reservoirs (*meso-reservoirs*) to equilibrium. That is to say, our density matrix follows the

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Lindblad equation of the following form:

$$\begin{aligned}
\frac{d\rho}{dt} &= -i[H, \rho] + D(\rho) \\
D(\rho) &= \sum_{k,\alpha,m} \left(2L_{k,\alpha,m}\rho L_{k,\alpha,m}^\dagger - \{L_{k,\alpha,m}^\dagger L_{k,\alpha,m}, \rho\} \right) \\
H &= H_S + H_L + H_R + V \\
H_S &= -\sum_{j=1}^{n-1} \left(t_j c_j^\dagger c_{j+1} + (h.c.) \right) + \sum_{j=1}^n U_j c_j^\dagger c_j \\
H_\alpha &= \sum_{k=1}^K \epsilon_k^\alpha a_{k\alpha}^\dagger a_{k\alpha}, \quad \alpha = L, R \\
V &= \sum_{k=1}^K \left(v_k^L a_{kL}^\dagger c_1 + v_k^R a_{kR}^\dagger c_n \right) + (h.c.) \\
L_{k,\alpha,1} &= \sqrt{\Gamma_{k,\alpha,1}} a_{k\alpha}, \quad L_{k,\alpha,2} = \sqrt{\Gamma_{k,\alpha,2}} a_{k\alpha}^\dagger \\
\Gamma_{k,\alpha,1} &= \gamma_k^\alpha (1 - F_\alpha(\epsilon_k)), \quad \Gamma_{k,\alpha,2} = \gamma_k^\alpha F_\alpha(\epsilon_k) \quad ,
\end{aligned} \tag{2.1}$$

where c_j is the annihilation operator of system fermions, $a_{k,\alpha}$ is that of reservoir fermions with wave number k , t_j is the nearest neighbor hopping, U_j is the on-site potential, v_k^α is the coupling between the system and reservoirs, and $F_\alpha(\epsilon) = (e^{\beta_\alpha(\epsilon - \mu_\alpha)} + 1)^{-1}$ are Fermi distributions, with inverse temperatures β_α and chemical potentials μ_α , while $[\cdot, \cdot]$ and $\{\cdot, \cdot\}$ denote the commutator and anti-commutator, respectively. The parameter γ_k^α determines the strength of the coupling to the super-reservoirs and needs to be fine-tuned in order to ensure the applicability of the model.¹⁾ We stress that our model does not rely on the usual weak-coupling assumption needed for the physical derivation of the Lindblad master equation,⁴⁾ thus γ_k^α do not need to be small parameters.

§3. Conservation laws

3.1. Particle conservation

In this section, we discuss conservation of particle number and energy. We focus first on the particle current. Let $n_j = c_j^\dagger c_j$ and $n_k^\alpha = a_{k\alpha}^\dagger a_{k\alpha}$ ($\alpha = L, R$), then, with time derivatives that can be casted as

$$\begin{aligned}
\frac{dn_j}{dt} &= J_{j-1}^P - J_j^P, \quad (1 \leq j \leq n-1) \\
J_0^P &\equiv i \sum_k v_k^L (a_{kL}^\dagger c_1 - c_1^\dagger a_{kL}) \equiv \sum_k j_k^L \\
J_j^P &\equiv -it_j (c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j), \quad (1 \leq j \leq n-1) \\
J_n^P &\equiv -i \sum_k v_k^R (a_{kR}^\dagger c_n - c_n^\dagger a_{kR}) \equiv \sum_k j_k^R
\end{aligned}$$

$$\begin{aligned}\frac{dn_k^L}{dt} &= -j_k^L + D(n_k^L) \\ \frac{dn_k^R}{dt} &= j_k^R + D(n_k^R) \quad ,\end{aligned}\tag{3.1}$$

where the dissipative parts $D(n_k^\alpha)$ are given by

$$\begin{aligned}D(n_k^\alpha) &= -2\Gamma_{k,\alpha,1} n_k^\alpha + 2\Gamma_{k,\alpha,2}(\mathbf{1} - n_k^\alpha) \\ &= -2\gamma_k^\alpha n_k^\alpha + 2\gamma_k^\alpha F_\alpha(k)\mathbf{1} \quad .\end{aligned}\tag{3.2}$$

By taking the expectation value in the *nonequilibrium steady state* (NESS) $\langle \cdot \rangle = \text{tr}(\cdot \rho(t \rightarrow \infty))$, we obtain

$$\begin{aligned}\sum_k \langle j_k^L \rangle &= \langle J_0 \rangle = \langle J_1 \rangle = \cdots = \langle J_{n-1} \rangle = \langle J_n \rangle = \sum_k \langle j_k^R \rangle \equiv J^P \\ \langle j_k^L \rangle &= \langle D(n_k^L) \rangle, \quad \langle j_k^R \rangle = -\langle D(n_k^R) \rangle \quad .\end{aligned}\tag{3.3}$$

Thus, the particle current from the left meso-reservoir to the system $\sum_k \langle j_k^L \rangle$ is equal to the current from the system to the right meso-reservoir $\sum_k \langle j_k^R \rangle$, and there is no particle loss due to the existence of the Lindblad dissipators. Moreover, we have

$$J^P = \sum_k \langle D(n_k^L) \rangle = -\sum_k \langle D(n_k^R) \rangle, \tag{3.4}$$

and it follows

$$J^P = 2 \sum_k \gamma_k^L \{ \langle n_k^L \rangle - F_L(k) \} = -2 \sum_k \gamma_k^R \{ \langle n_k^R \rangle - F_R(k) \} \quad . \tag{3.5}$$

This expression can be understood as a generalization of the Landauer formula for the current between the meso-reservoirs and the super-reservoirs. Moreover, if γ_k^α is independent of k , the total differences of charge densities from their equilibrium state values are proportional to $(1/\gamma^\alpha)$.

3.2. Energy conservation

We now turn our attention to the conservation of energy. Casting the local energy density as

$$\begin{aligned}H_j &\equiv -\left(t_j c_j^\dagger c_{j+1} + t_j c_{j+1}^\dagger c_j\right) + U_j c_j^\dagger c_j, \quad (1 \leq j \leq n) \\ c_{n+1} &\equiv 0 \quad ,\end{aligned}\tag{3.6}$$

their time derivatives are

$$\begin{aligned}\frac{dH_j}{dt} &= J_{j-1}^E - J_j^E, \quad (1 \leq j \leq n-2) \\ J_0^E &\equiv U_1 J_0^P + i \sum_k v_k^L t_1 (c_2^\dagger a_k - a_k^\dagger c_2) \\ J_j^E &\equiv i t_j t_{j+1} (c_j^\dagger c_{j+2} - c_{j+2}^\dagger c_j) + U_{j+1} J_j^P, \quad (1 \leq j \leq n-2)\end{aligned}$$

$$\begin{aligned}
\frac{dH_{n-1}}{dt} &= J_{n-2}^E - J_{n-1}^E - \tilde{J}_n^E \\
J_{n-1}^E &\equiv U_n J_{n-1}^P \\
\tilde{J}_n^E &\equiv i \sum_k v_k^R t_{n-1} (b_k^\dagger c_{n-1} - c_{n-1}^\dagger b_k) \\
\frac{dH_n}{dt} &= J_{n-1}^E - J_n^E \\
J_n^E &\equiv U J_n^P = iU \sum_k v_k^R (c_n^\dagger a_{kR} - a_{kR}^\dagger c_n) \\
\frac{dV_L}{dt} &= -J_0^E + J_{L \rightarrow V}^E + D(V_L) \\
\frac{dV_R}{dt} &= J_n^E + \tilde{J}_n^E - J_{V \rightarrow R}^E + D(V_R) \\
J_{L \rightarrow V}^E &\equiv i \sum_k \epsilon_k^L v_k^L (a_k^\dagger c_1 - c_1 a_k^\dagger) \equiv \sum_k \epsilon_k^L j_k^L \\
J_{V \rightarrow R}^E &\equiv -i \sum_k \epsilon_k^R v_k^L (b_k^\dagger c_n - c_n b_k^\dagger) \equiv \sum_k \epsilon_k^R j_k^R \\
\frac{dH_L}{dt} &= -J_{L \rightarrow V}^E + D(H_L) \\
\frac{dH_R}{dt} &= J_{V \rightarrow R}^E + D(H_R) \quad , \tag{3.7}
\end{aligned}$$

where the dissipative terms $D(V_\alpha)$ and $D(H_\alpha)$ are given by

$$\begin{aligned}
D(V_L) &= - \sum_k \gamma_k^L v_k^L (a_{kL}^\dagger c_1 + c_1^\dagger a_{kL}) \\
D(V_R) &= - \sum_k \gamma_k^R v_k^R (a_{kR}^\dagger c_n + c_n^\dagger a_{kR}) \\
D(H_\alpha) &= 2 \sum_k \gamma_k^\alpha \epsilon_k (F_L(k) \mathbf{1} - n_k^\alpha) \quad . \tag{3.8}
\end{aligned}$$

By taking average with respect to the NESS we obtain

$$\begin{aligned}
\langle J_0^E \rangle &= \langle J_1^E \rangle = \dots = \langle J_{n-2}^E \rangle = \langle J_{n-1}^E \rangle + \langle \tilde{J}_n^E \rangle = \langle J_n^E \rangle + \langle \tilde{J}_n^E \rangle \\
i \sum_k v_k^L t_1 \langle c_2^\dagger a_k - a_k^\dagger c_2 \rangle &= i \sum_k t_{n-1} v_k^R \langle a_{kR}^\dagger c_{n-1} - c_{n-1}^\dagger a_{kR} \rangle \\
\langle D(H_L) \rangle + \langle D(V_L) \rangle &= -\langle D(H_R) \rangle - \langle D(V_R) \rangle \quad . \tag{3.9}
\end{aligned}$$

Although, the total particle current at the two meso-reservoirs is conserved, i.e., $\sum_k \langle j_k^L \rangle = \sum_k \langle j_k^R \rangle$, the particle current distributions are not the same, i.e.,

$$-2\gamma_k^L \{ \langle n_k^L \rangle - F_L(k) \} = \langle j_k^L \rangle \neq \langle j_k^R \rangle = 2\gamma_k^R \{ \langle n_k^R \rangle - F_R(k) \} \quad . \tag{3.10}$$

Thus, the ingoing energy current at the left hand side is not equal to the outgoing energy current at the right hand side, i.e., $\sum_k \epsilon_k^L \langle j_k^L \rangle \neq \sum_k \epsilon_k^R \langle j_k^R \rangle$.

In our case,

$$\langle D(H_L) \rangle = \sum_k \epsilon_k \langle j_k^L \rangle = 2 \sum_k \epsilon_k v_k^L \operatorname{Im} \langle c_1^\dagger a_k \rangle \quad (3.11)$$

and

$$\langle D(V_L) \rangle = -2 \sum_k \gamma_k^L v_k^L \operatorname{Re} \langle c_1^\dagger a_k \rangle \quad (3.12)$$

are not conserved separately, and it induces the difference of the energy current from left meso-reservoir to system and that from system to right meso-reservoir. Namely, the following four statements are deeply connected:

- (1) Different amount of energy is dissipated at left and right $\langle D(V_L) \rangle \neq -\langle D(V_R) \rangle$.
- (2) The energy current from left meso-reservoir and that to right meso-reservoir are different $\langle J_{L \rightarrow S}^E \rangle \neq \langle J_{S \rightarrow R}^E \rangle$.
- (3) The particle current distribution of two reservoirs are different $\langle j_k^L \rangle \neq \langle j_k^R \rangle$.
- (4) The particle distribution of two reservoirs are different $\langle n_k^L \rangle \neq \langle n_k^R \rangle$.

§4. Numerical results

As discussed in,¹⁾ expectation values with respect to the NESS are easily obtained by solving $2n \times 2n$ dimensional Sylvester equation. In this section, we discuss the transport properties of periodic, Fibonacci and disordered chains at NESS.

We study monoatomic ($t_j = t$), diatomic ($t_{2j-1} = t_A$, $t_{2j} = t_B$), Fibonacci, and disordered chains. The Fibonacci chain is constructed by first taking $n = 3$ and setting $t_1 = t_A$, $t_2 = t_B$ constituting the first generation, and then inductively replacing t_A by $t_A t_B$ and t_B by t_A . For instance, the second generation yields $n = 4$ and $t_1 = t_A$, $t_2 = t_B$, $t_3 = t_A$; the third generation yields $n = 6$ and $t_1 = t_A$, $t_2 = t_B$, $t_3 = t_A$, $t_4 = t_A$, $t_5 = t_B$, and so on. Alternatively, one can construct n -th generation by concatenating $(n - 2)$ -th generation after $(n - 1)$ -th generation.

For disordered chains, we take t_j from a uniform distribution in $[t - \delta, t + \delta]$.

To make things simple, we have set $U_j = U$, $v_k^L = v_k^R = v$ and $\gamma_k^L = \gamma_k^R = \gamma$ for numerical results. As discussed in,¹⁾ v should be smaller than γ , and we have set $\gamma = 0.1$, $v = 0.03$, $\epsilon_1 = -20$, $\epsilon_K = 20$, $K = 200$, and $\mu_L = -\mu_R = \mu$, unless specified differently.

We have checked that reservoirs are close enough to equilibrium and satisfy conservation law (3.5). We show the j dependence of occupation density $\langle n_j \rangle$ and n dependence of the particle current J^P in Fig. 1 (monoatomic $t = 3$ and diatomic chain $t_A = 3$, $t_B = 6$), Fig. 2 (Fibonacci chain $t_A = 3$, $t_B = 6$), and Fig. 3 (disordered chain $t = 3$, $\delta = 0.3, 2.9$). For monoatomic, diatomic, and Fibonacci chains, red dots represent $\gamma = 0.1$, and blue dots represent $\gamma = 1$.

One can see that the occupation density of periodic chains is constant except at the edge, and the particle current reaches non-zero constant^{*)} for large n , and

^{*)} the constant depends on the parity of system size n for diatomic chains

the transport is ballistic. Red dots ($\gamma = 0.1$) show a small deviation since the interaction between the system and the reservoirs is relatively small. The Fibonacci chain shows large fluctuations in occupation and system size dependence of the particle current, though it is very robust against the change of γ . For small disordered chains ($t = 3$, $\delta = 0.3$), the particle current decreases linearly as a function of system size, and the occupation shows a linear profile. For disordered chains ($t = 3$, $\delta = 2.9$), occupation profile has a kink shape and the particle current decreases nearly exponentially.

For sufficiently small thermal and chemical gradients, the particle and the heat current, defined as $J_Q \equiv J_E - \bar{\mu}J_P$ ($\bar{\mu} = (\mu_L + \mu_R)/2$), depend linearly on the external gradients as^{5),6),7)}

$$\begin{aligned} J_Q &= L_{QQ}\Delta\beta - L_{QP}\beta\Delta\mu, \\ J_P &= L_{PQ}\Delta\beta - L_{PP}\beta\Delta\mu, \end{aligned}$$

where $\Delta\beta \equiv \beta_R - \beta_L$ and $\Delta\mu \equiv \mu_R - \mu_L$. The second law of thermodynamics imposes definite-positiveness of the matrix of Onsager coefficients \mathbf{L} , which implies $L_{QQ} \geq 0$ and $L_{PP} \geq 0$, and if the dynamics is time-reversible, the Onsager's reciprocity relation $L_{PQ} = L_{QP}$ holds.

In Fig. 4 we consider the Fibonacci chains with $t_A = 3$ and show the dependence of various properties of \mathbf{L} on the other hopping parameter t_B . Fig. 4(a) shows the t_B dependence of all Onsager coefficients. One sees that all coefficients are positive, where we remark that possibility of negative off-diagonal elements were discussed in.¹⁾

Fig. 4(b) shows the thermoelectric figure-of-merit $ZT \equiv L_{PQ}L_{QP}/\det\mathbf{L}$ ⁸⁾ for diatomic and Fibonacci chains. One sees that diatomic chains have larger ZT than the Fibonacci chains for the most parameter regimes.

Fig. 4(c) shows the γ dependence of $|L_{PQ}/L_{QP} - 1|$ for diatomic and Fibonacci chains. We see that the Onsager reciprocity is roughly linearly broken by increasing γ for the diatomic chains. It is very similar for the Fibonacci chains, however here the asymmetry has a cusp shape near $\gamma \sim 0.03$, and one should be more careful with the choice of γ in order to have (approximate) time-reversal symmetry.

§5. Conclusions

We have established a conservation law for particle number, and a conservation law for the sum of energy current along the chain and dissipation at the boundaries of the chain. The conservation laws are valid for generic one-dimensional chains connected to meso-reservoirs, which described by bilinear hamiltonian.

As an application, we have studied the transport properties of monoatomic, diatomic, quasi-periodic, and disordered chains. We have observed wide fluctuations in the occupation and the system size dependence of the particle current for the Fibonacci chain. For the disordered chain, we have observed linearly or exponentially decreasing currents. The occupation was shown to have either linear profile or kink shape, respectively.

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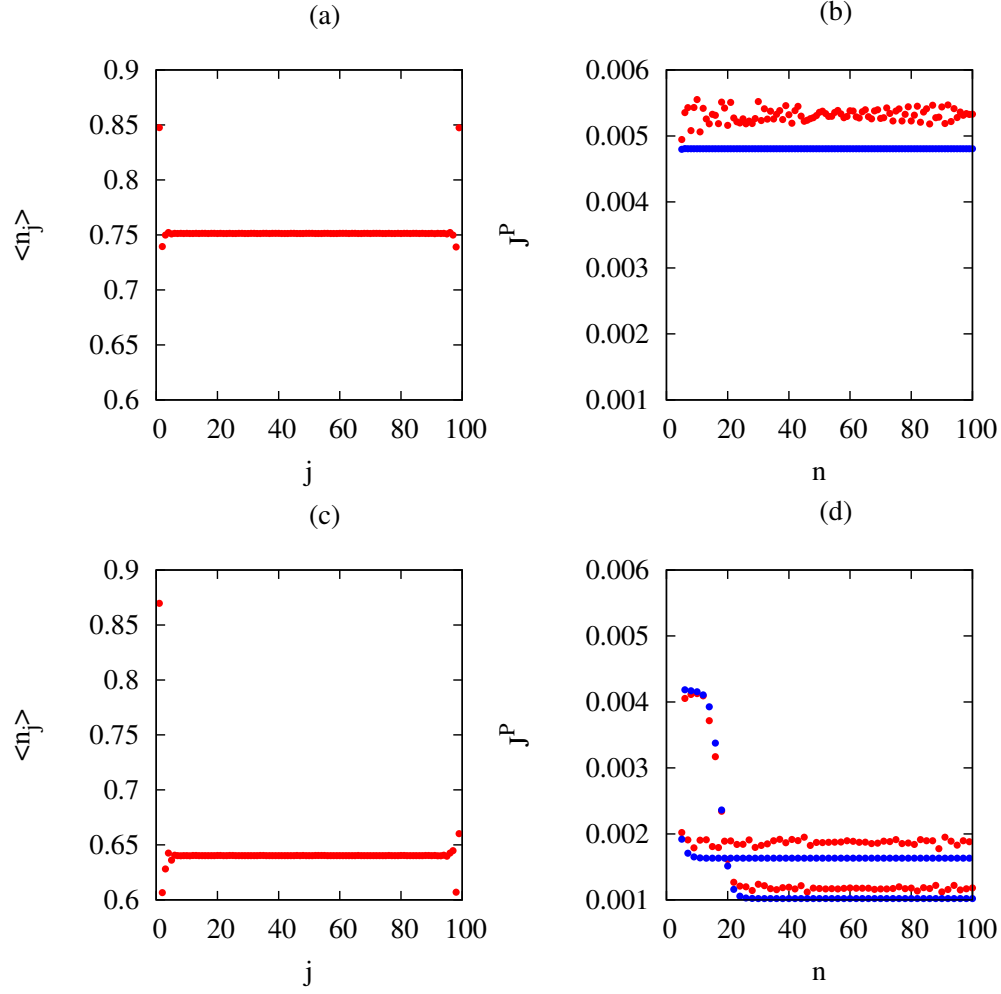


Fig. 1. (Color online) Panel (a) and (c) show position (j) dependence of occupation density n_j for (a) monoatomic chain, and (c) diatomic chain. Panels (b) and (d) show n dependence of the particle current J^P for (b) monoatomic chain, and (d) diatomic chain (red: $\gamma = 0.1$, blue: $\gamma = 1$)

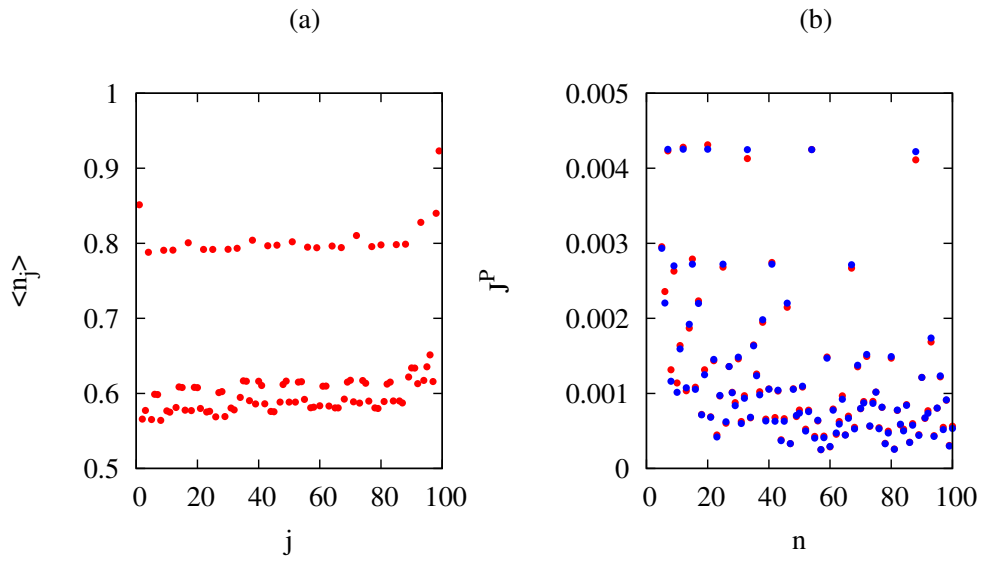


Fig. 2. (Color online) Panel (a) shows j dependence of occupation density n_j for the Fibonacci chain. Panel (b) shows chain size (n) dependence of the particle current J^P for the Fibonacci chain (red: $\gamma = 0.1$, blue: $\gamma = 1$)

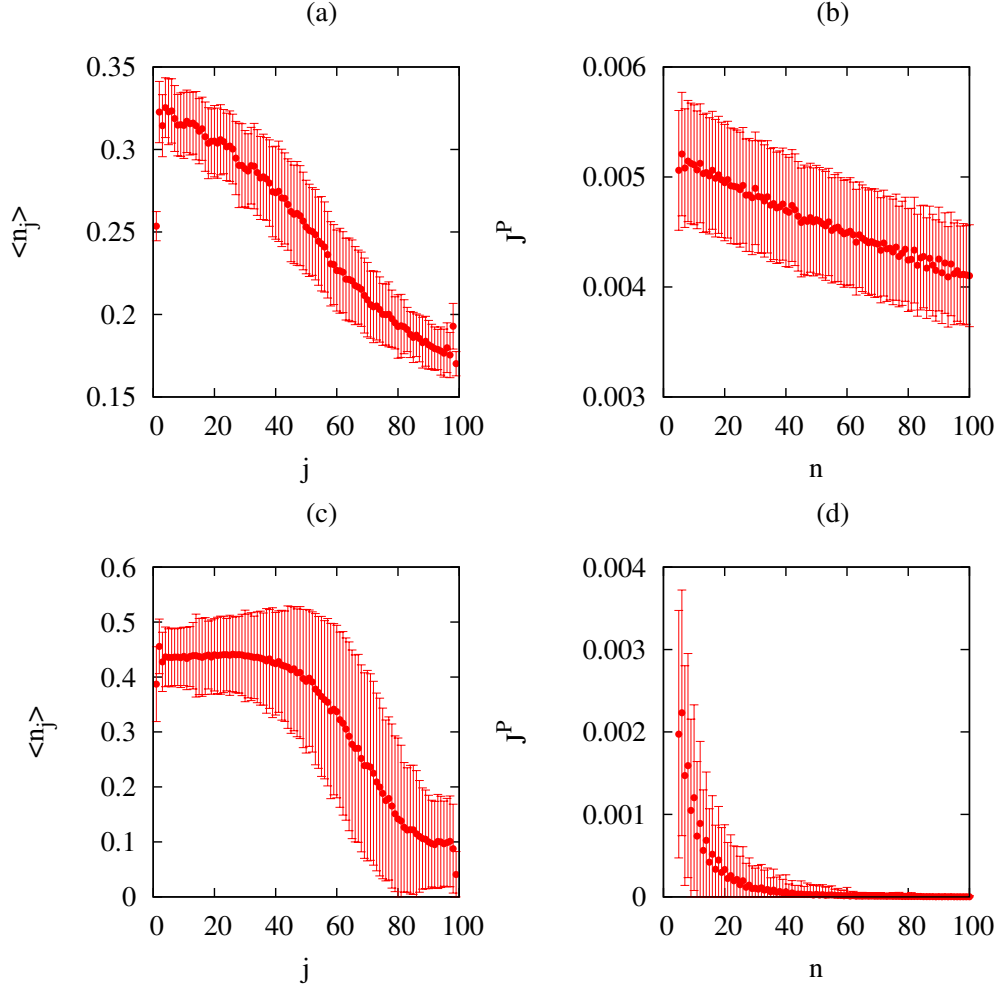


Fig. 3. (Color online) Panel (a) and (c) show j dependence of occupation density n_j for disordered chains. Panel (b) and (d) show n dependence of the particle current J^P for disordered chains. (a) and (c) is for $t = 3$, $\delta = 0.3$, and (b) and (d) is for $t = 3$, $\delta = 2.9$

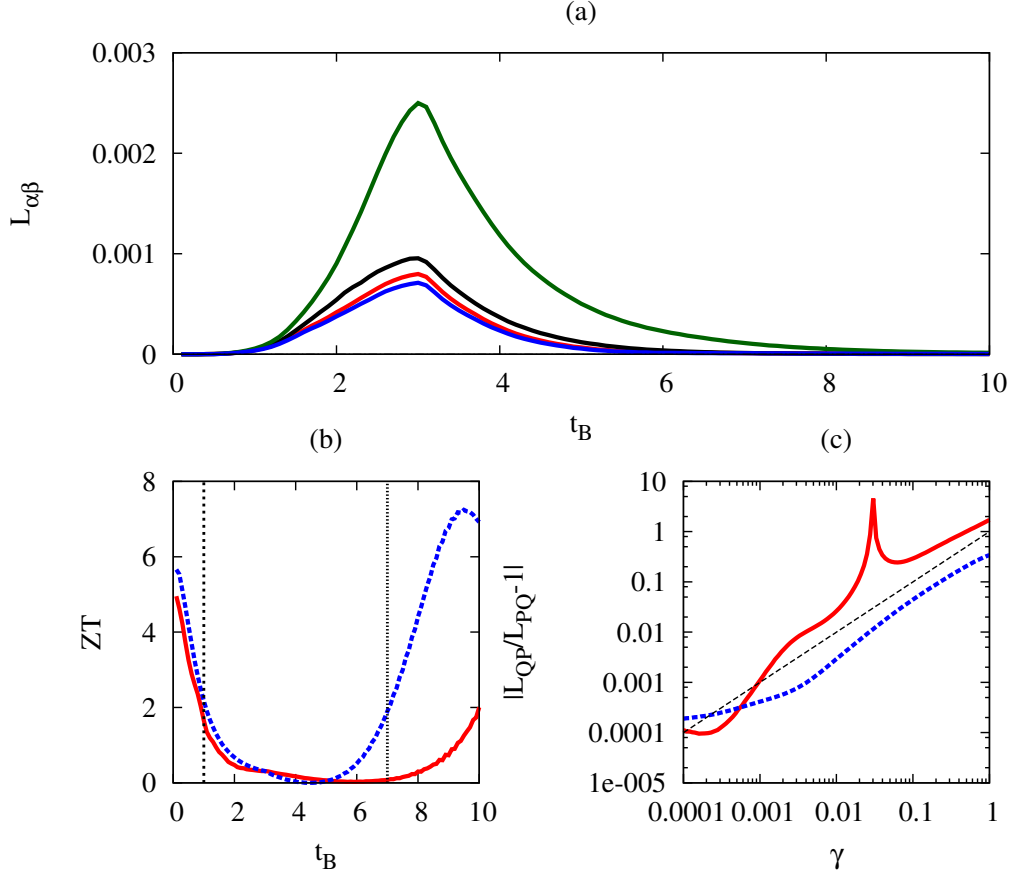


Fig. 4. (Color online) Panel (a) shows t_B dependence of the Onsager coefficients (color code: L_{QP} - red, L_{PP} - black, L_{QQ} - green, L_{PQ} - blue) for the Fibonacci chains. Panel (b) shows t_B dependence of ZT for diatomic (blue) and Fibonacci chains (red). Hoppings t_A are chosen as $t_A = 3$. For diatomic chains, they have exponentially small current outside $t_b \in [1, 7]$ indicated in the figure. Panel (c) shows the γ dependence of asymmetry $L_{QP}/L_{PQ} - 1$ for diatomic (blue) and Fibonacci (red) chains (dashed line indicates linear growth). t_A and t_B are chosen as $t_A = 3$, $t_B = 6$.